New Approach for a Data Engine Suitable for Process Calculations: Uncertainties and Process Design Quality

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Optimized thermodynamic model parameter databases are the cornerstone for the creation of models for process calculations. In this paper we describe the statistical tools and the general characteristics of a new database that collects the necessary model parameters for process calculations and simulations. This new database was created based on evaluated data only, with special considerations towards consistency of pure component and thermodynamic equilibrium data, extensive empirical and semi-empirical quality tests of derived models and comprehensive documentation and retrieval facilities for every piece of information stored in the system. The new thermodynamic model parameter database, VIRTUAL, provides users of chemical process calculations with high quality, extensively tested and consistent model parameters based on carefully screened experimental data, ranging from simple pure component temperature independent data to pure component temperature dependent data and thermodynamic equilibrium parameters for mixture modeling.